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# The Equation of State of LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-ox

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The Equation of State of LLM-105  
(2,6-diamino-3,5-dinitropyrazine-1-oxide)  
San Antonio, TX, United States  
March 1, 2015 through March 6, 2015

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## The Equation of State of LLM-105 (2,6-diamino-3,5-dinitropyrazine-1-oxide)

March 4, 2015

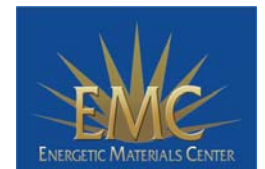


APS March Meeting, San Antonio TX

**Joseph M. Zaug, Elissaios Stavrou, and Bora Kalkan**

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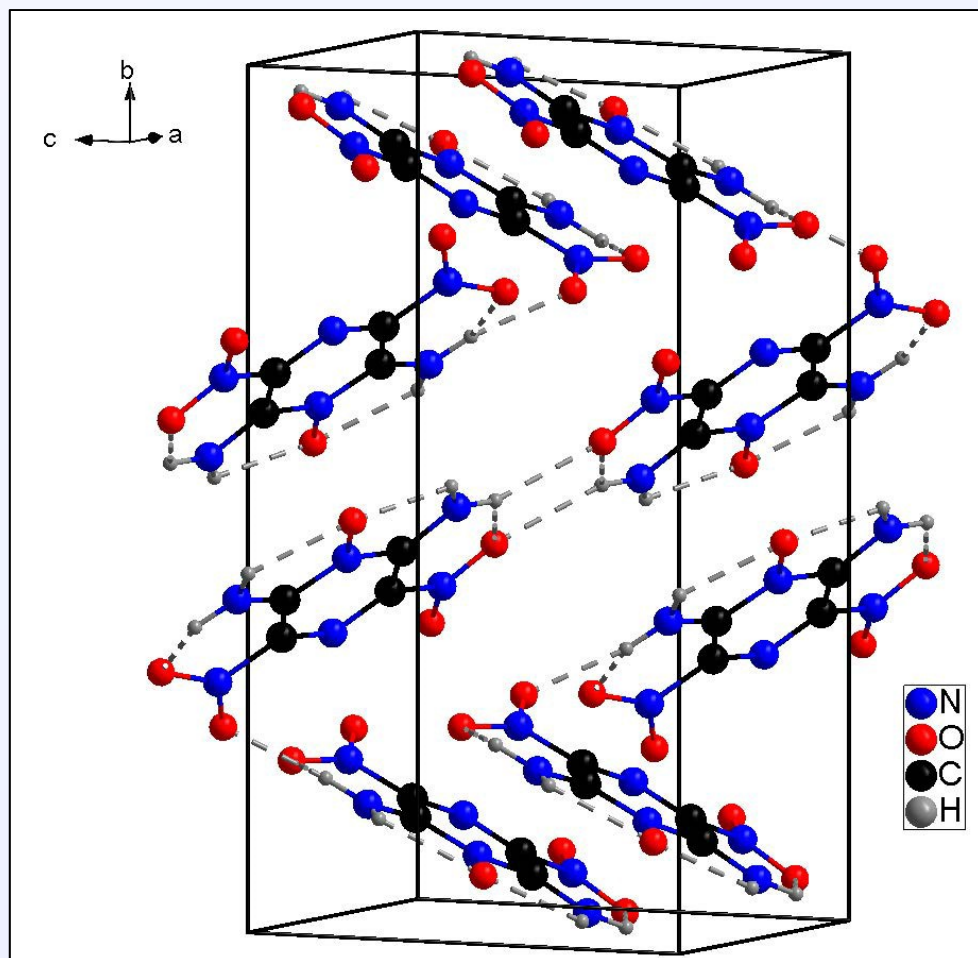
Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551  
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LLM-105 has a high density, detonation velocity,  
and is relatively difficult to initiate



### Ambient Pressure Representation of LLM-105



Monoclinic structure (SG: P21/n (14) )

Long-range H-bonding network

Theoretical results indicate phase transitions at 8, 17, 25, 42 GPa<sup>1</sup>

Theoretical results also indicate ambient phase stability to 45 GPa<sup>2</sup>

Previous Exp. work extends to 6 GPa<sup>3</sup>

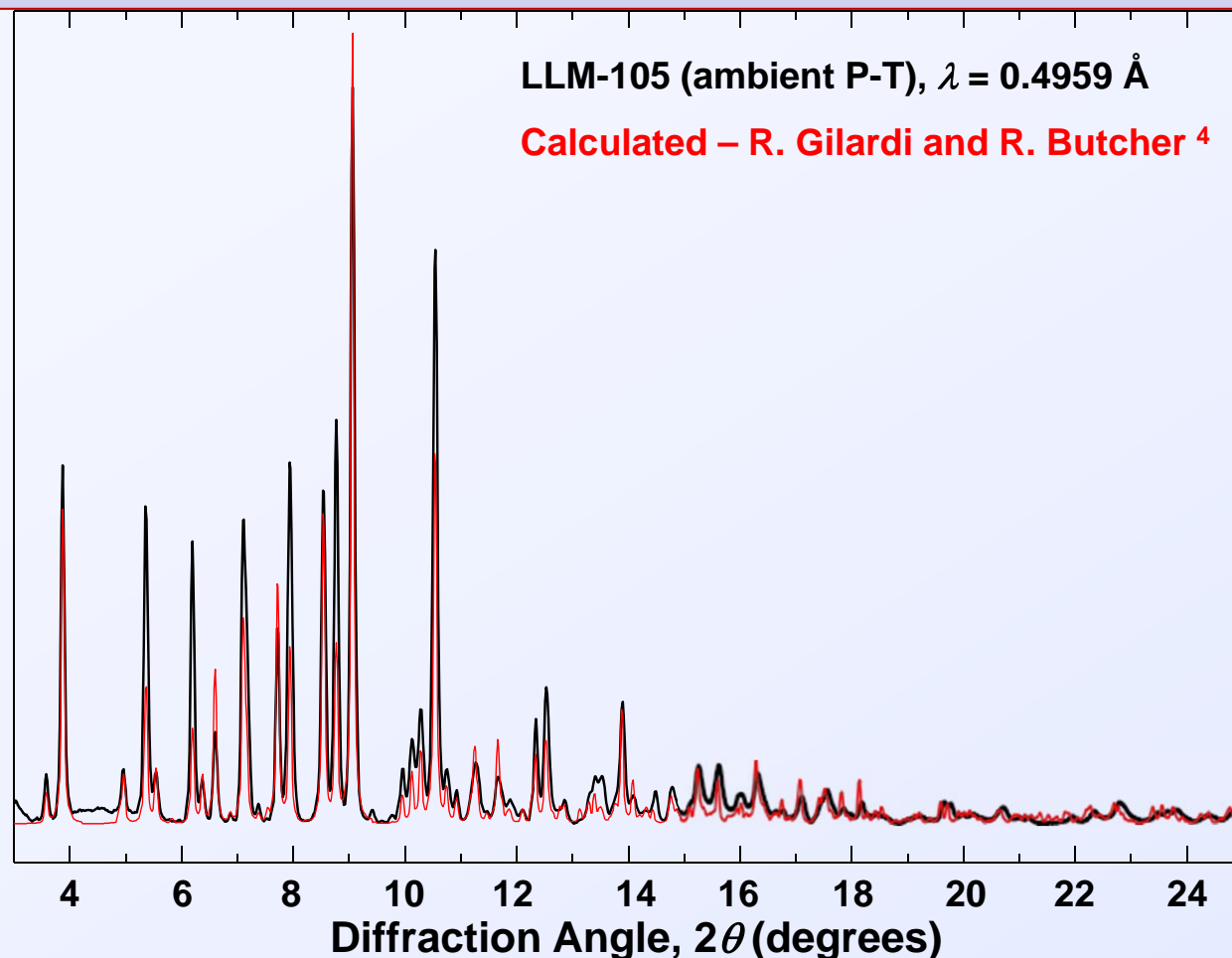
1. Q. Wu, C. Yang, Y. Pan, F. Xiang, Z. Liu, W. Zhu, and H. Xiao,  
*Journal of Molecular Modeling* **19**, 5159 (2013).
2. M. R. Manaa, I.-F. W. Kuo, and L. E. Fried,  
*J. Chem. Phys.* **141**, 064702 (2014).
3. J. C. Gump, C. A. Stoltz, B. P. Mason, B. G. Freedman, J. R. Ball, and S. M. Peiris,  
*J. Appl. Phys.* **110**, 073523 (2011).



# LLM-105 Powder Diffraction Bragg Peak Positions Match Well with Single Crystal X-ray Results



## Ambient Pressure X-ray Powder Diffraction Pattern - LLM-105



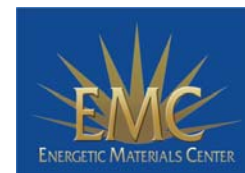
## Experimental Details

Ground powder  
Silicone oil PTM  
Au & Ruby P sensors  
400  $\mu\text{m}$  diamond culets  
Re gasket  
  
XRD experiments  
LBNL/ALS on BL 12.2.2  
 $\sim 10 \mu\text{m}$  FW-HM spot  
60s exposure per site  
FIT2D for integration  
GSAS LeBail Refinements

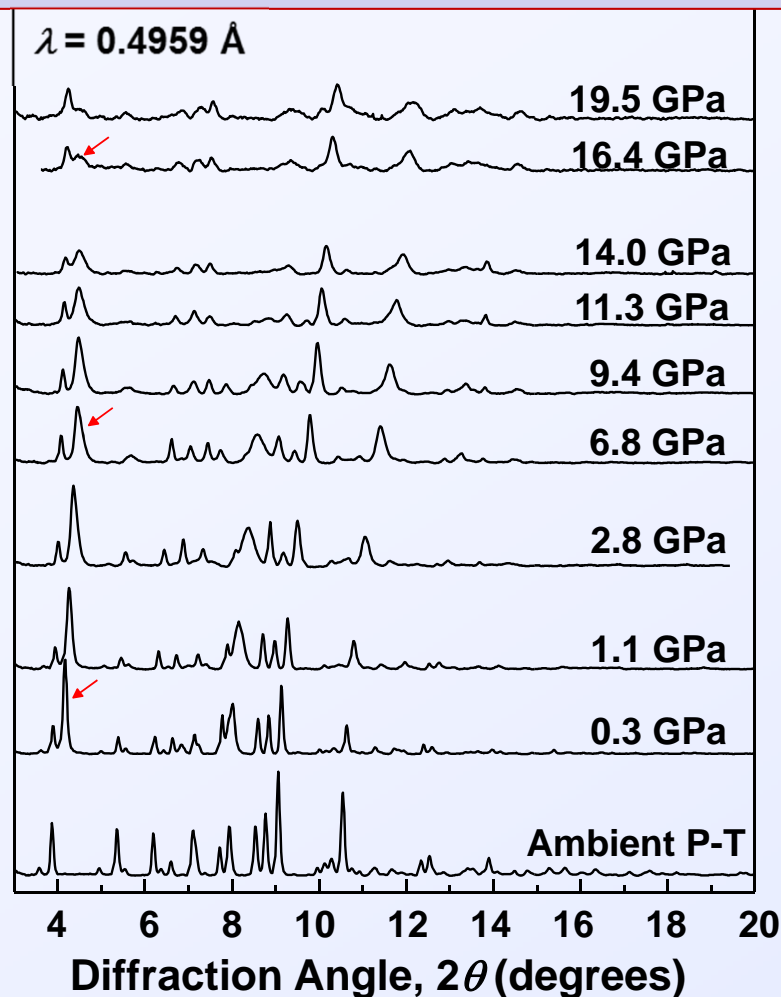
4. R. D. Gilardi and R. J. Butcher, *Acta Crystallographica Section E-structure Reports*, Online 57, o657 (2001).



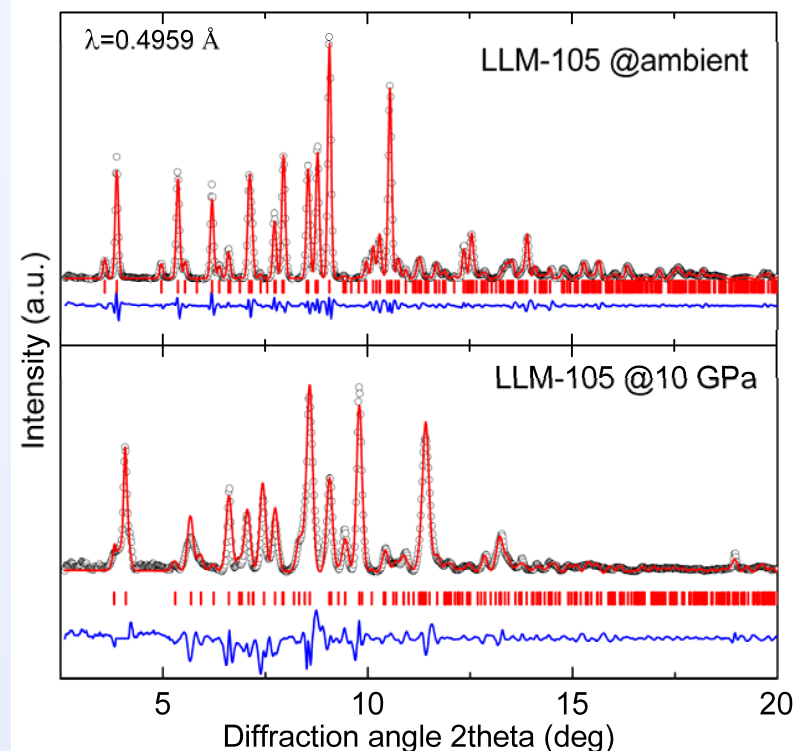
# Pressure Dependent Powder Diffraction Patterns Do Not Reveal a Structural Phase Transition



## Pressure Dependent Diffraction Patterns



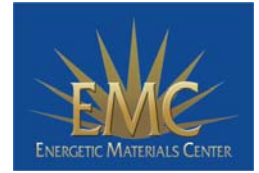
## LeBail Powder Diffraction Refinements



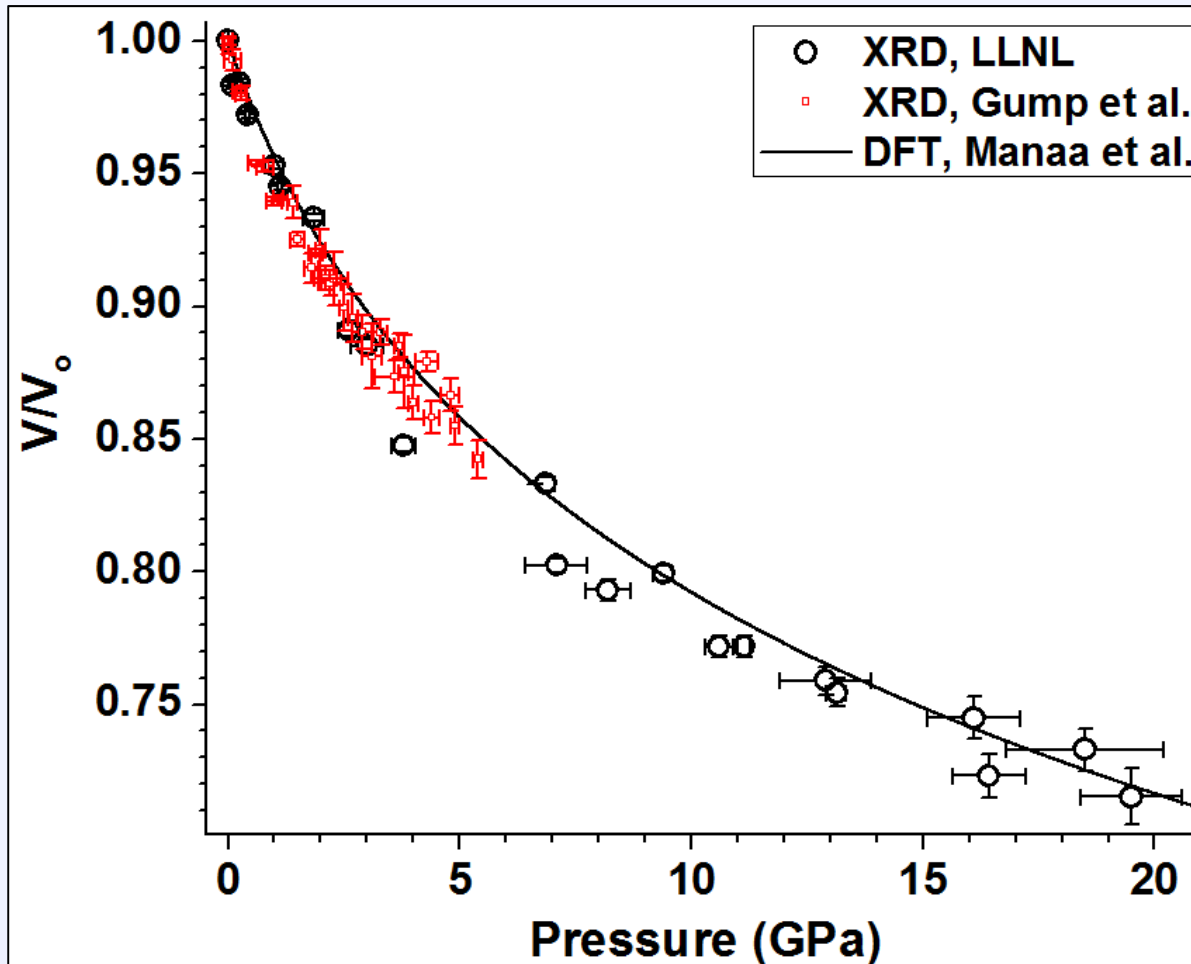
With exception to one high d-spacing peak, (See: red arrow), all patterns index well to the monoclinic structure (SG: P21/n (14) )



# The Experimental LLM105 P-V EOS Matches Well to Recent Dispersion Corrected DFT Results



## P-V EOS Comparison to Gump et al. and Manaa et al.



## EOS Param. Comparisons

Weighted 3<sup>rd</sup>-order

Birch-Murnaghan model

LLNL XRD | DFT | Gump et al.

$V_0$  ( $\text{\AA}^3$ ) 750.1 741.0 746.3

$K_0$  (GPa) 11.8 19.7 10.2

$K'_0$  17.8 7.1 23.4

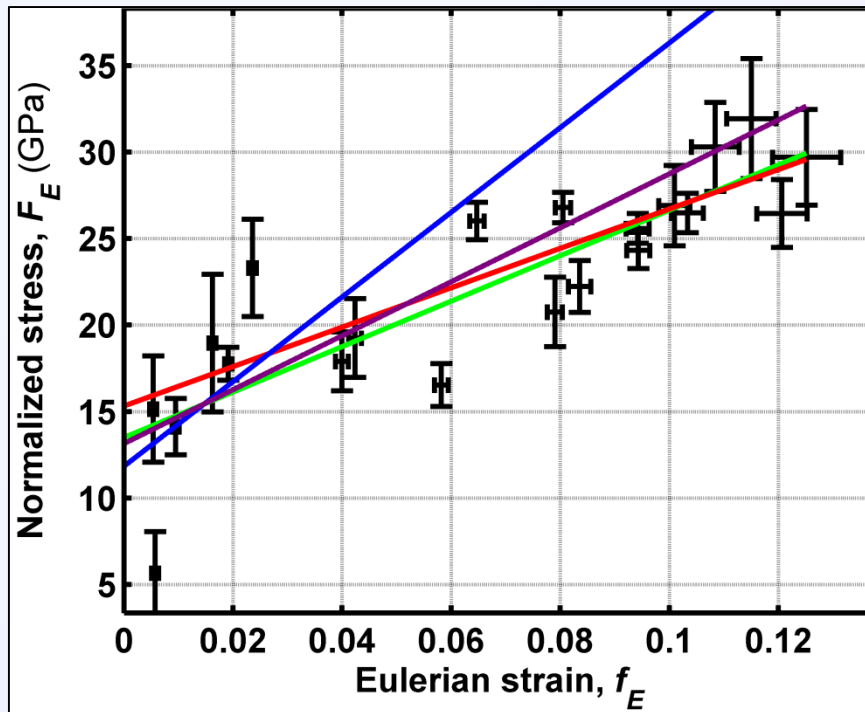
Single Crystal  $V_0 = 748.2 \text{ \AA}^3$



# The EOS Model That Best Approximates our P-V EOS Data is the 1<sup>st</sup>-order $F$ - $f$ model

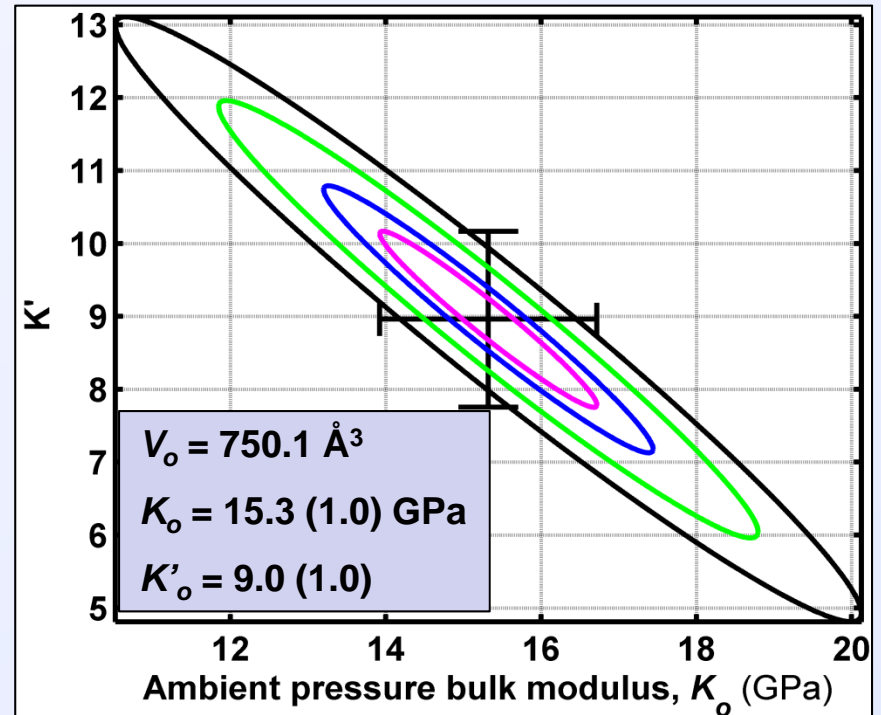


$F$ - $f$  EoS Model Fits



LLM105 cold-compression data fit to a first-order  $F$ - $f$  model. The green line represents an unweighted fit and the red line is an experimentally weighted fit. The blue line is from a 3<sup>rd</sup> order B-M fit and the violet line is a Vinet EOS model fit.

$F$ - $f$  1<sup>st</sup>-order Confidence Ellipses



Confidence ellipses for the weighted  $F$ - $f$  fit. The magenta colored ellipse is 0.607- $\sigma$ , blue is 1- $\sigma$ , green is 2- $\sigma$ , and the black ellipse is 3- $\sigma$ .

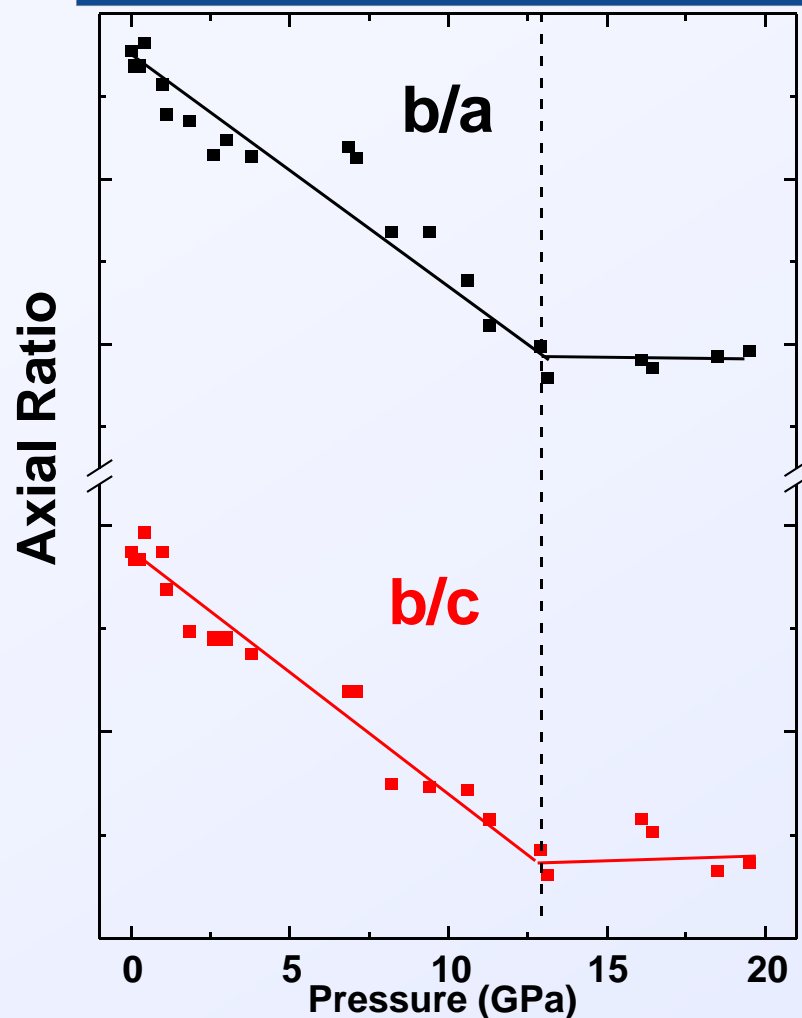




# The Pressure Dependent Axial Ratios Reveal the Onset of Inter-Sheet Stiffening at ~ 13 GPa



Pressure dependent axial ratios



The b-axis is the most compressible

The change in slope at ~ 13 GPa signals a significant change in the relative compressibility along the b-axis (it matches the compressibility of the a and c axes)

At ~ 13 GPa, the inter-sheet distance becomes nearly the same as intra-molecular distances



# Questions?

